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Title: Experience with ENDF60 and QA of a Continuous-energy Library

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SUBJECT: Experience with ENDF60 and QA of a Continuous-energy Library

The continuous-energy neutron data library ENDF60 was released at LANL and at RSICC (Radiation Safety Information Computational Center) in the fall of 1994 (LA-12891 and errata). As you may recall, the QA procedures followed for this library were different than previously released libraries. Valuable experience has been gained over the past two years with the ENDF60 library, and the purpose of this memorandum is to briefly document the results of a more standardized QA process and the results of applying this process to the ENDF60 library. Some information in this memorandum will therefore be redundant with previous documentation (XTM: SCF-96-328).

This QA process only took a moderate amount of time (~ a week), it is in the understanding of identified problems and the resolution of them that significant amounts of time are spent in the complete QA process. At the most recent MCNP BoD meeting (XTM: JSH-96-357), consensus was reached to pursue the release of an ENDF61 library which would completely replace ENDF60 and that no further QA efforts should be expended on ENDF60. The information contained below will be useful in examining the new ENDF61 library. At the end of the memorandum, a short discussion of the internal QA performed by NJOY is included.

General Information for ENDF60
The original ENDF60 library contained data for 124 nuclides, 2 of which were later removed from distribution at LANL and at RSICC. The data for Am-242 ground state and Np-238 were removed due to the evaluations being very incomplete, no reaction data except elastic scattering were available above 11 keV (XTM: SCF-96-145). This library was based on ENDF/B-VI evaluations through Release 2 and contained approximately 66 new evaluations and 56 translated evaluations relative to ENDF/B-V Release 0. Exact numbers are difficult to ascertain as the source for each data file was not documented at the time. The revised Table 1 from LA-12891 contains the most current and accurate information.

What Files should be Archived for each Library
For completeness the following files should be archived for each new MCNP library on CDROM. A utility on the Crays, CFSAR, can be used to copy everything under one CFS subdirectory to another in an automated manner. This is useful in copying the

source evaluations and PENDF tapes for archiving purposes. The PENDF tapes must be stored on separate CDROMs from the other information due to their size.

Type 1 data library or the individual data files
Evals: source evaluations for each nuclide/data file
Fiche/NJOY_output: the NJOY interpretive output listing for each data file
Programs: any programs specific to this library used in processing and their associated input and output files
PENDF tapes: the NJOY PENDF tapes and files used in the NJOY processing

Charged Particle Production MT's for ENDF60

Until very recently, NJOY did not have the ability to create the total charged particle production MT information (MT=203-207) that had been added in a post-processing sense by the Data Team in the past. ENDF60 therefore does not contain any total charged particle production information, and this part of the QA process did not need to be performed (XTM: SCF-96-199).

Verification of Correct Resonance Data Processing

The neutron resonance fitting code SAMMY may be used to verify that the data in the resonance region has been processed correctly (XTM: SCF-96-104). This is typically only used on when working with multitemperature data files, and when problems are suspected. If the source evaluation contains data in file 3 that is added/subtracted from the calculated resonance data, this information is not available to SAMMY and the comparisons will not be exact. No comparisons with SAMMY were performed for the ENDF60 library.

Reaction Thresholds

The code CHECKTHRESH was run on the type 1 ENDF60 library. CHECKTHRESH.F compares threshold energies with kinematic thresholds for negative Q-value reactions. The code calculates the kinematic threshold as

$$\mathrm{K.T.} = \frac{-Q * (\mathrm{AWR} + 1)}{\mathrm{AWR}} \quad ,$$

where AWR is the atomic weight ratio and Q is the Q-value. If the actual threshold on the library is lower than the kinematic threshold, the code outputs this information along with the magnitude of the discrepancy, the law specified for the secondary neutrons, and the line number on the type 1 library containing the problem energy value. Currently, while incorrect values for the thresholds may exist, it is likely that MCNP will only experience a fatal error for distributions using LAW=3. The code also identifies the largest threshold error detected.

Five nuclides were determined to have threshold errors; Gd-155, Gd-156, Gd-160, Ta-181, and Cf-249. In particular, the threshold error for Gd-160 would require some thought to fix in the ENDF60 library and may cause problems for future libraries. Table 1 details the threshold error information given by CHECKTHRESH for these nuclides.

Secondary Neutron Distributions

The code CHECKND_NEUT was run on ENDF60. The code CHECKND_NEUT.F analyzes various aspects of secondary neutron energy distributions using LAW=4 or LAW=44 on a type 1 library. The code verifies that interpolation schemes 1 or 2 are used, and identifies any negative probability density functions if found. The code checks to see if any secondary neutrons can be produced with energies greater than the energy of the incident neutron (for fission the code takes no corrective action). The code will actually fix two specific types of problems, 1) it changes negative probability density functions to zero and 2) it corrects for secondary neutron energies greater than incident where appropriate and renormalizes. It then creates a new data library if any modifications have been made.

Nine nuclides were shown to have problems in the ENDF60 library; Fe-57, Ni-61, Y-89, W-182, W-184, W-186, Au-197, Pb-206, Pb-207, Pb-208. Additionally, one must be careful of the (n,n'α) reaction (MT=22) for Bi-209 which has a positive Q-value of 3.1440 MeV. This does indeed represent physical upscatter and should be allowed. Table 2 lists the error messages produce by CHECKND_NEUT for ENDF60.

Secondary Photon Distributions

The code CHECKND was run on ENDF60, and no problems with the secondary distributions were detected. CHECKND.F analyzes various aspects of secondary photon energy distributions using LAW=4 or LAW=44 on a type 1 library. It informs the user if all the secondary photon energies are discrete (informational only), and if there are any negative discrete energies at adjacent incident neutron energies. The code also checks the number of discrete energies at adjacent incident neutron energies, and notifies the user if such a problem is found (this will cause errors in MCNP). If the number of discrete secondary photon energies are the same for adjacent incident neutron energies, the code verifies that the photon energies are the same as well (this will cause errors in MCNP).

However, NJOY still lacks the capability to produce angular dependent secondary distributions for photons (they are all created as isotropic distributions). The C and O evaluations specify non-isotropic secondary photon distributions and therefore this data is missing from ENDF60. In the past, the Data Team has added this information to the data file after the NJOY processing was complete.

Data Files using the MT=5 Reaction

The code CHECK5 reads a type 1 data library and analyzes data files which contain MT=5 data. MT=5 is used to combine many reactions, including fission, into one and is used primarily at higher incident neutron energies (>20 MeV). CHECK5.F prints out the threshold energy and first (energy, yield) pair for secondary neutrons. In particular, the code is checking for the following situation; if the threshold for the MT=5 cross section is lower than the threshold for the MT=5 secondary neutron production (as given by the first (e,y) pair), then the first yield must be 0, or MCNP will use the data inappropriately at all energies less than the first (e,y) pair. All information is written to an output file, and the user must review the file for the above situation. The data files in the ENDF60 library contained no MT=5 data.

Examination of the Reaction Cross-Sections
The code XDATAP6 (soon to be renamed XSPLOT) was run to produce plots of all reaction cross section data in addition to the total, elastic, total absorption, and neutron heating data for each nuclide. These plots were then examined to identify any questionable data. Questionable data may indeed be representative of the evaluation or a result of the processing from an evaluation to data file. Typically, one would follow-up on each one of these items and reach a decision concerning its validity. This follow-up has not been performed for this library, and the questionable data listed in Table 3 should be examined in the QA of the new ENDF61 library. Figures 1-5 illustrate some of the types of questionable data that may be encountered; elastic cross section, negative heating, and very poor evaluation data in general. Additionally, it is useful to use the compare option in XDATAP6 to compare cross section data for the new data file to previously available data (compare a .60c to .50c data for a particular nuclide). This type of comparison has also not been performed to a great extent for the ENDF60 library.

There is another mechanism for comparing cross-section data numerically, WHALE.F (XTM: NDK-95-253). This code allows the user to compare cross section data that has been group averaged (groups and weight functions as defined by user). WHALE can handle ENDF evaluations, PENDF tapes from NJOY, type 1 data files, and DTF format multigroup data, and can make comparisons between any of these types of data. It is often useful to make this type of comparison when preparing a MENDF multigroup library, or when changes to an evaluation should not have produced any changes in the cross section data for a given nuclide. Comparison between ENDF60 data and the source evaluations were not performed, but WHALE was used extensively to compare the DTF files for MENDF6 with the data in ENDF60 for the relevant nuclides.

NJOY Internal QA
NJOY has incorporated a number of internal QA/consistency checks over the past couple of years. These may not have been available during the production of the ENDF60 library, but many were available when NJOY (version 94.10) was used to produce the interpretive output listings of the data files. This output listing is much like the older fiche outputs, and are currently stored on CDROM. The information from the internal NJOY checks is written at the beginning of the output files. Unfortunately, there is no common error message that one could use to ‘grep’ all of the output files at one time. Table 4 lists the NJOY error messages that were produced. As discussed in a previous memorandum (XTM: SCF-95-301), it is hoped that as many of the above QA procedures as possible can eventually be worked into the internal NJOY checking process.

From Table 4, it is clear that the threshold errors were detected accurately by NJOY. These type of threshold errors are now corrected by NJOY automatically during processing. If NJOY is being used to produce the interpretive output listing for libraries which it did not process, as was done for the ENDL92 library, It would be helpful if future error messages included the full complement of significant digits, and highlighted when additional problems in changing the energy values would occur such as for Gd-160. The bad cumulative probability errors detected for Bi-209 are a result of a minor NJOY bug which has since been corrected.

The error message for F-19 concerning the incorrect frame-of-reference arises because of a special feature of the F-19 data and is in fact not in error. There are two secondary neutron energy distributions given for the (n,2n) reaction, MT=16, for F-19. These are processed as two separate MT values each having 1/2 the cross section for this reaction. The two processed MT values for this reaction are 6 and 46, indicated as the (n,1/2*1) and (n,2/2*1) reactions by NJOY respectively. Both have TYR values of +2, indicating two neutrons are given off for each 1/2 cross section in the lab frame so that the total secondary neutron production is preserved.

Table 1: Threshold Errors in the ENDF60 Data Library

```
64155.60c mt= 28 q= -7.63200 egiven= 7.6816900000000E+00 should be  7.6816900880254E+00 diff= 1.1E-08 law= 9 line=1218878
64156.60c mt= 16 q= -8.53650 egiven= 8.5917200000000E+00 should be  8.5917227605881E+00 diff= 3.2E-07 law= 9 line=1233298
64160.60c mt= 22 q= -1.00400 egiven= 1.0103300000000E+00 should be  1.0103322674437E+00 diff= 2.2E-06 law= 9 line=1273813
                                  big trouble -- next energy in grid = 1.0103320000000E+00
73181.60c mt= 58 q= -0.62000 egiven= 6.2345590000000E-01 should be  6.2345596432553E-01 diff= 1.0E-07 law= 3 line=1327919
73181.60c mt= 59 q= -0.72000 egiven= 7.2401330000000E-01 should be  7.2401337792642E-01 diff= 1.1E-07 law= 3 line=1327921
73181.60c mt= 60 q= -0.92500 egiven= 9.3015600000000E-01 should be  9.3015607580825E-01 diff= 8.2E-08 law= 3 line=1327924
73181.60c mt=103 q= -0.23870 egiven= 2.4003050000000E-01 should be  2.4003054626533E-01 diff= 1.9E-07 law= 2 line=1327909
98249.60c mt= 51 q= -0.06249 egiven= 6.2743000000000E-02 should be  6.2743057422856E-02 diff= 9.2E-07 law= 3 line=2239285
                                                   biggest change= 2.24426E-06
```

Table 2: Secondary Neutron Distribution Problems in ENDF60

	ZAID	MT	Incident Energy	Outgoing Energy
trouble:	26057.60c	91	einc= 2.00000E+01	eprimemax= 2.04480E+01
trouble:	28061.60c	91	einc= 2.00000E+01	eprimemax= 2.04026E+01
trouble:	39089.60c	91	einc= 3.20000E+00	eprimemax= 3.33200E+00
trouble:	74182.60c	91	einc= 3.00000E-01	eprimemax= 3.75000E-01
trouble:	74184.60c	91	einc= 5.00000E-01	eprimemax= 6.50000E-01
trouble:	74186.60c	91	einc= 3.00000E-01	eprimemax= 3.75000E-01
trouble:	79197.60c	91	einc= 1.00000E-01	eprimemax= 1.87500E-01
trouble:	82206.60c	91	einc= 2.00000E+01	eprimemax= 2.03110E+01
trouble:	82207.60c	91	einc= 2.00000E+01	eprimemax= 2.03100E+01
trouble:	82208.60c	91	einc= 2.00000E+01	eprimemax= 2.03091E+01

Table 3: Cross Section Data to be Further Checked

He-4	No absorption data
B-11	Abs. and photon production - thinning near 10 keV
C	Abs. near 10 keV
N-15	No photon prod. < 5.0 MeV
O-16	Abs. and photon prod. data
F-19	Photon prod. 100 keV, heating <1 eV and resonance region
Mg	Abs. near 1 MeV, negative heating
Si	Negative heating
P-31	Abs. and photon prod. 100 keV - 1 MeV
S-nat	Photon prod. around 900 keV
K-nat	Abs. and photon prod. 10 keV - 1 MeV
Ca-nat	Abs. and photon prod. 1-100 keV
Ti-nat	Negative heating
V-nat	Photon prod. ~30 keV
Fe-57	Elastic xs 300 keV- 1.5 MeV (see Figure 1)
Fe-58	Photon prod. 0.4-1 MeV
Ni-61	Elastic xs 0.5-1.0 MeV
Ni-62	Abs. and photon prod. ~ 10 keV
Ga-nat	Poor data in general
Y-89	Negative heating
Nb-93	Negative heating
Mo	Bad/Neg. heating (see Figure 2)
In	Negative heating
Cs-135	Very poor data (see Figure 3)
Cs-137	Very poor data
Ba-138	Negative heating
Eu-151	Bad/Neg. heating
Ta-181	Bad/Neg. heating
Ta-182	Abs. 0.3-1.0 MeV
W-183	Negative heating
W-184	Bad/Neg. heating
Au-197	Negative heating
Bi-209	Negative heating
Th-232	Negative heating
U-232	Elastic xs, 1-10 eV
Np-239	Very poor data
Pu-236	Very poor data (see Figure 4)
Pu-237	Very poor data (see Figure 5)
Pu-244	Very poor data
Pu-243	Very poor data
Cm-241	Very poor data
Cm-242	Negative heating
Cm-244	Elastic xs 1-10 eV
Cm-246	Elastic xs 100 eV
Cm-248	Elastic xs 1eV- 1keV
Cf-250	Very poor data
Cf-251	Very poor data
Cf-252	Very poor data

Table 4: Consistency Check Output from NJOY

```
check reaction thresholds against q values

CF98249.OUT:    threshold error:  6.274306E-02  6.274300E-02     (n,n*1)
GD64155.OUT:    threshold error:  7.681690E+00  7.681690E+00     (n,n*)p
GD64156.OUT:    threshold error:  8.591723E+00  8.591720E+00     (n,2n)
GD64160.OUT:    threshold error:  1.010332E+00  1.010330E+00     (n,n*)a
TA73181.OUT:    threshold error:  6.234560E-01  6.234559E-01     (n,n*8)
TA73181.OUT:    threshold error:  7.240134E-01  7.240133E-01     (n,n*9)
TA73181.OUT:    threshold error:  9.301561E-01  9.301560E-01     (n,n*10)
TA73181.OUT:    threshold error:  2.400305E-01  2.400305E-01     (n,p)

 check that main energy grid is monotonic

 check angular distributions for correct reference frame

F9019.OUT:    should be cm: (n,1/2*1)

 check angular distributions for unreasonable cosine values

 check energy distributions

BI83209.OUT: bad cumm. prob for (n,n')p    at   3.8160E+00  2.0000E+00
BI83209.OUT: bad cumm. prob for (n,n')d    at   8.9840E+00  4.0000E+00
BI83209.OUT: bad cumm. prob for (n,n')t    at   9.4690E+00  4.0000E+00

 check photon distributions
```

Figure 1: Elastic Cross Section for Fe−57

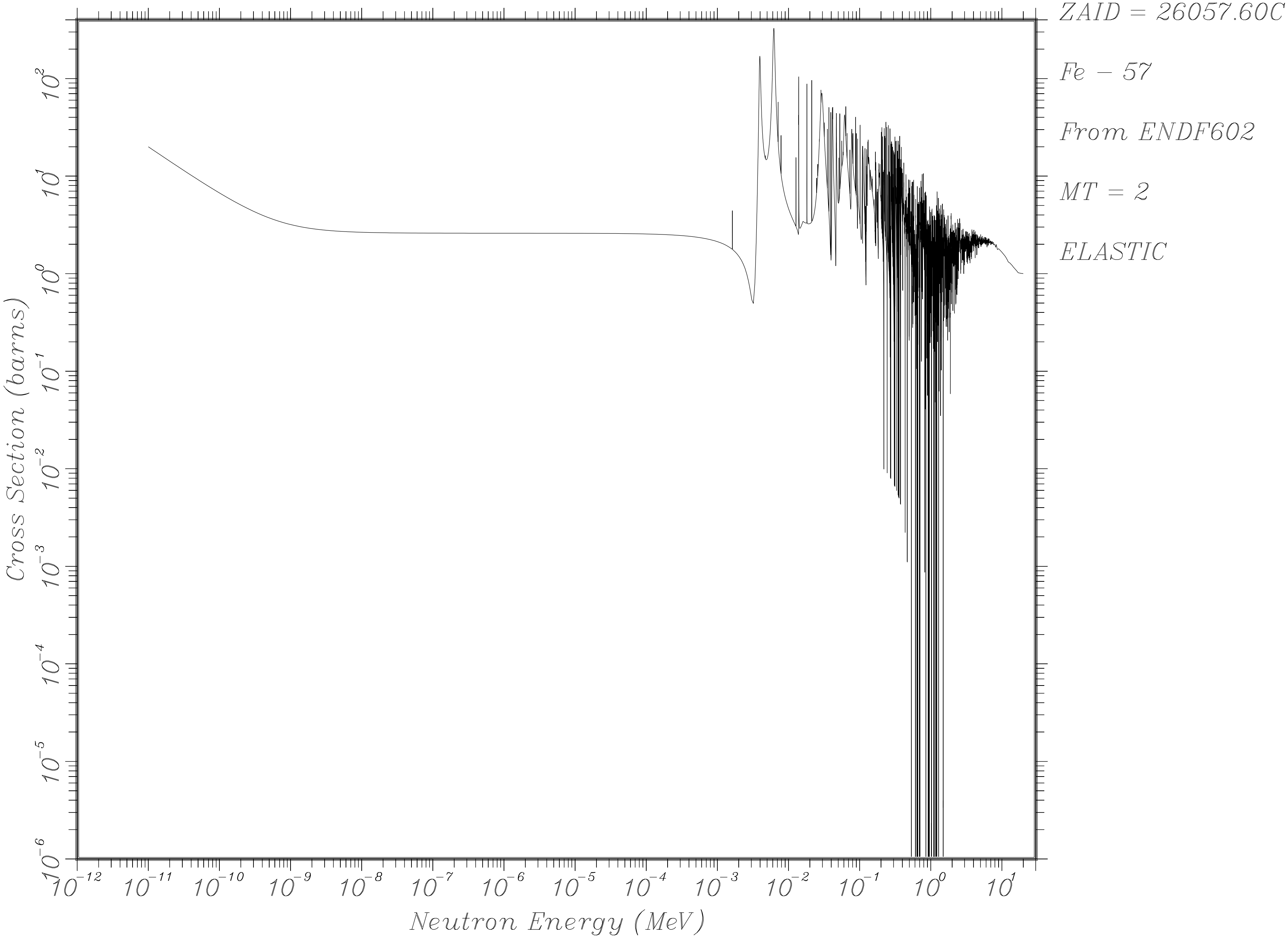


Figure 2: Heating Numbers for Natural Mo

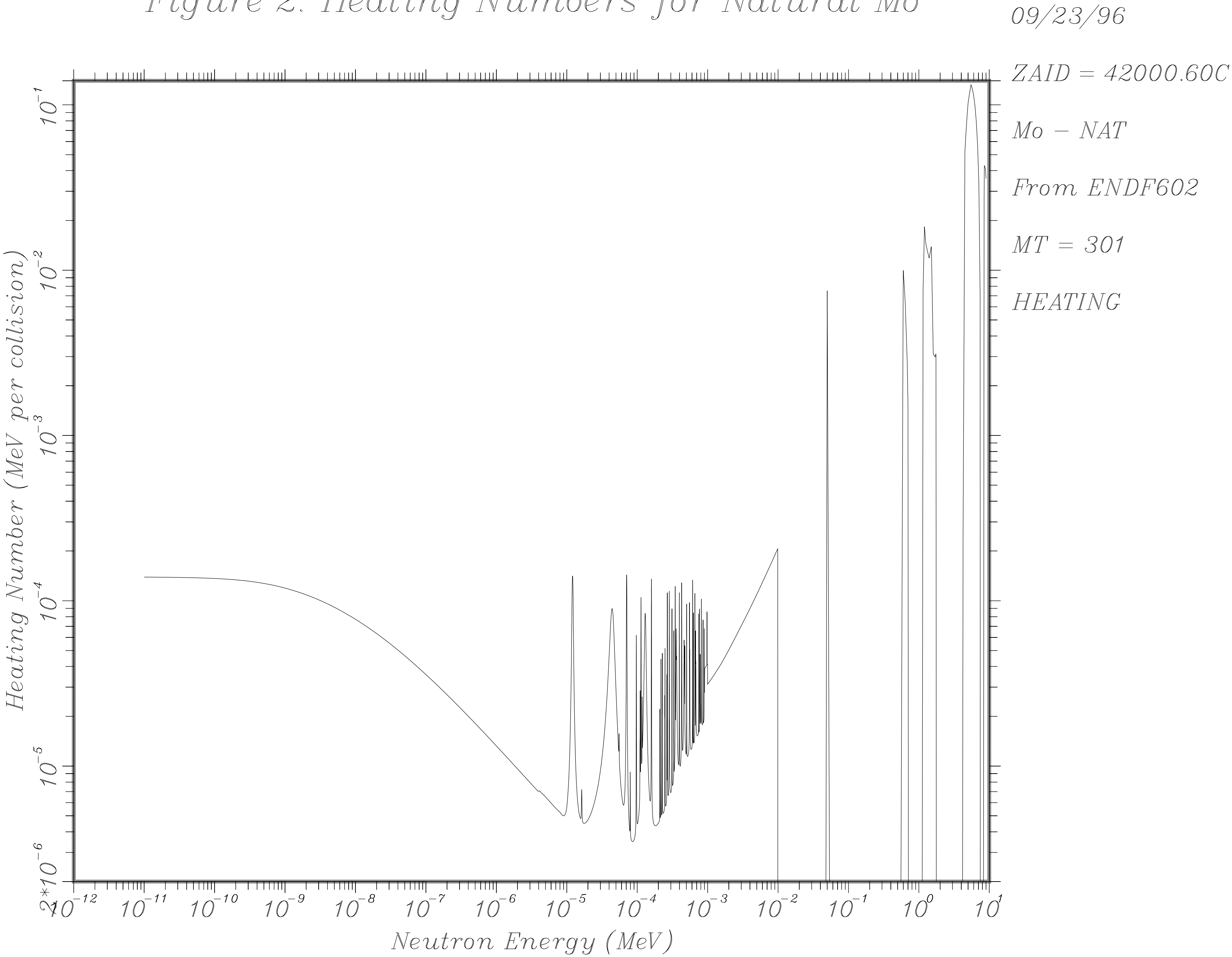


Figure 3: Total Cross Section for Cs–135

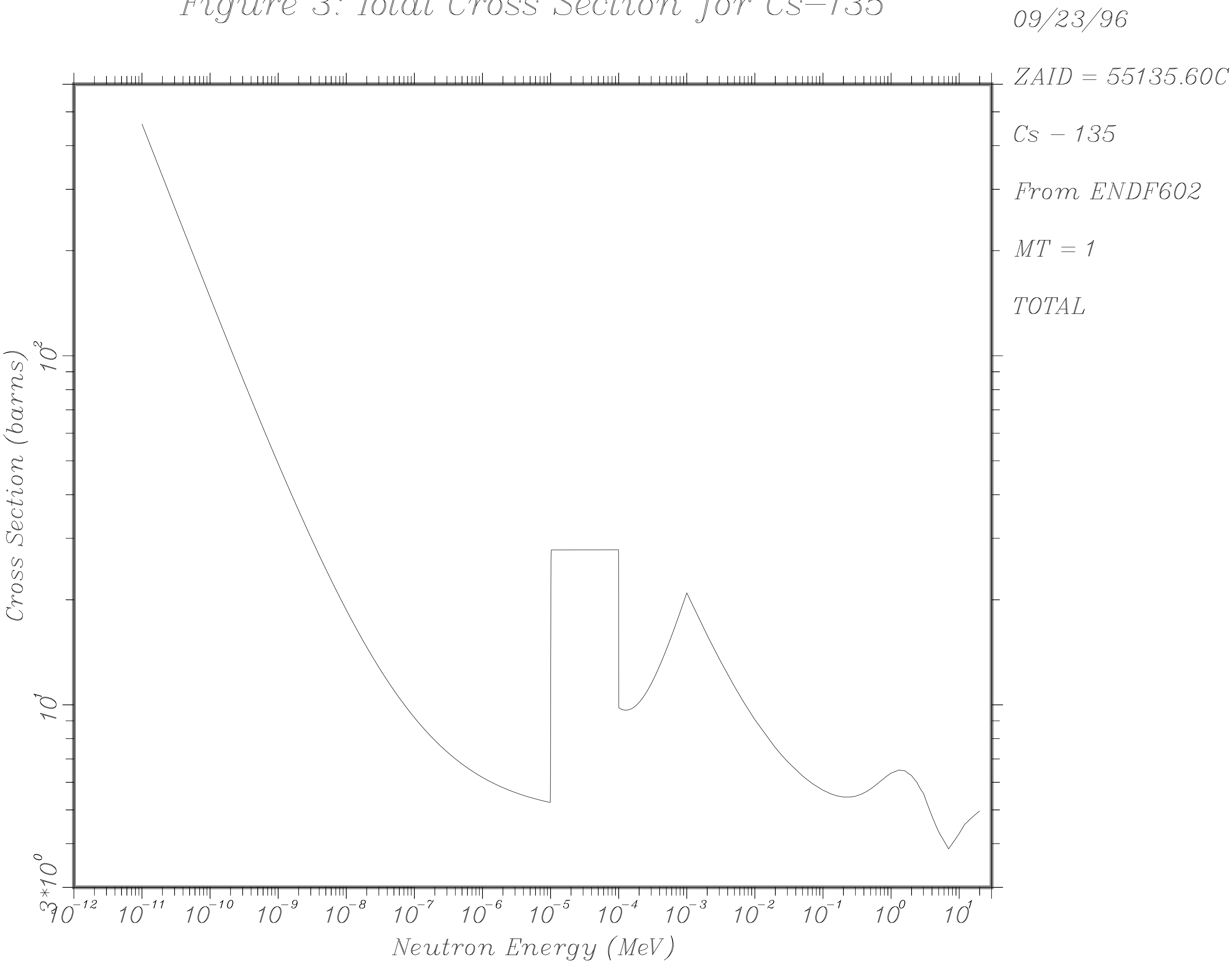
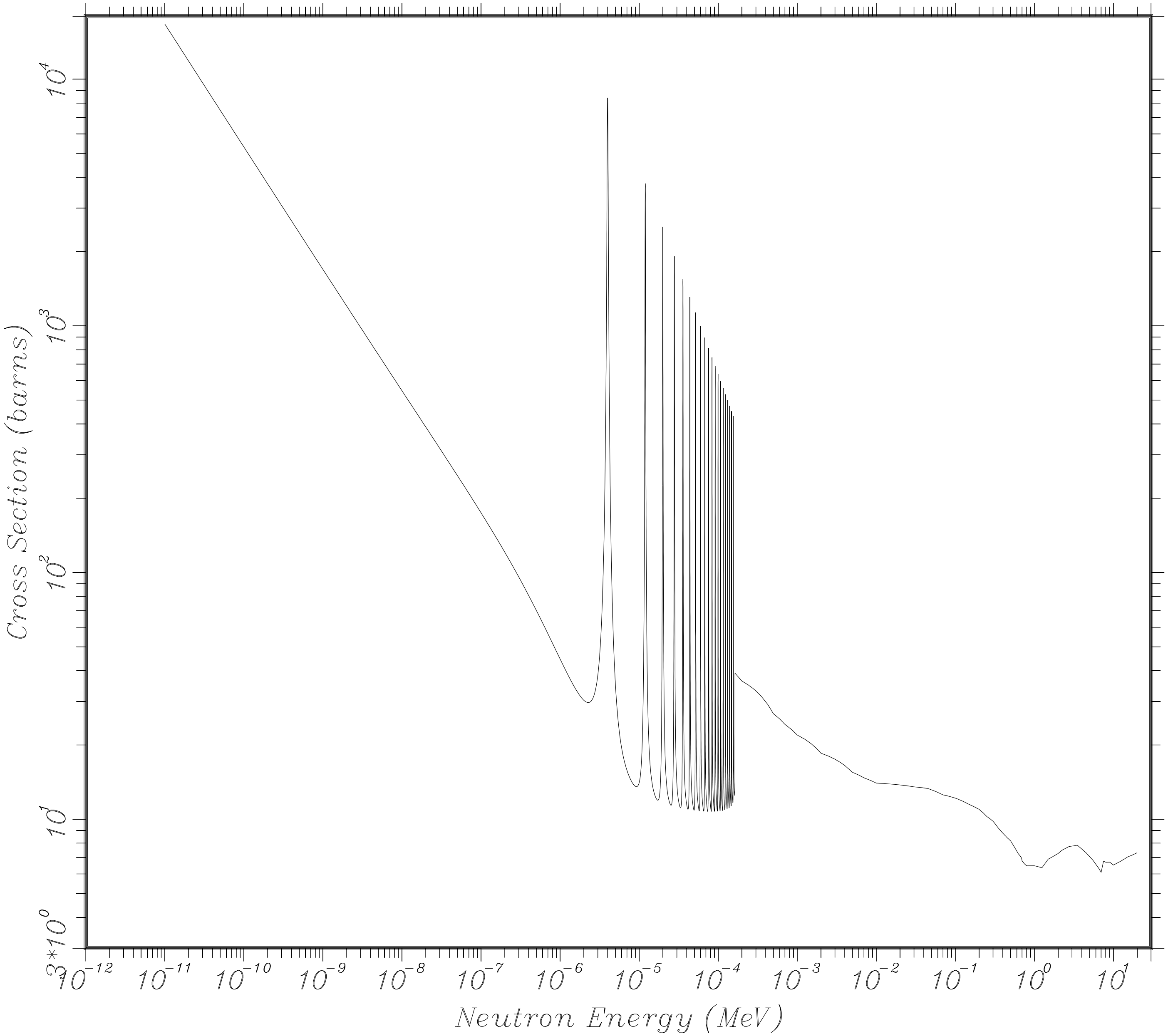


Figure 4: Total Cross Section for Pu-236



09/23/96

ZAID = 94236.60C

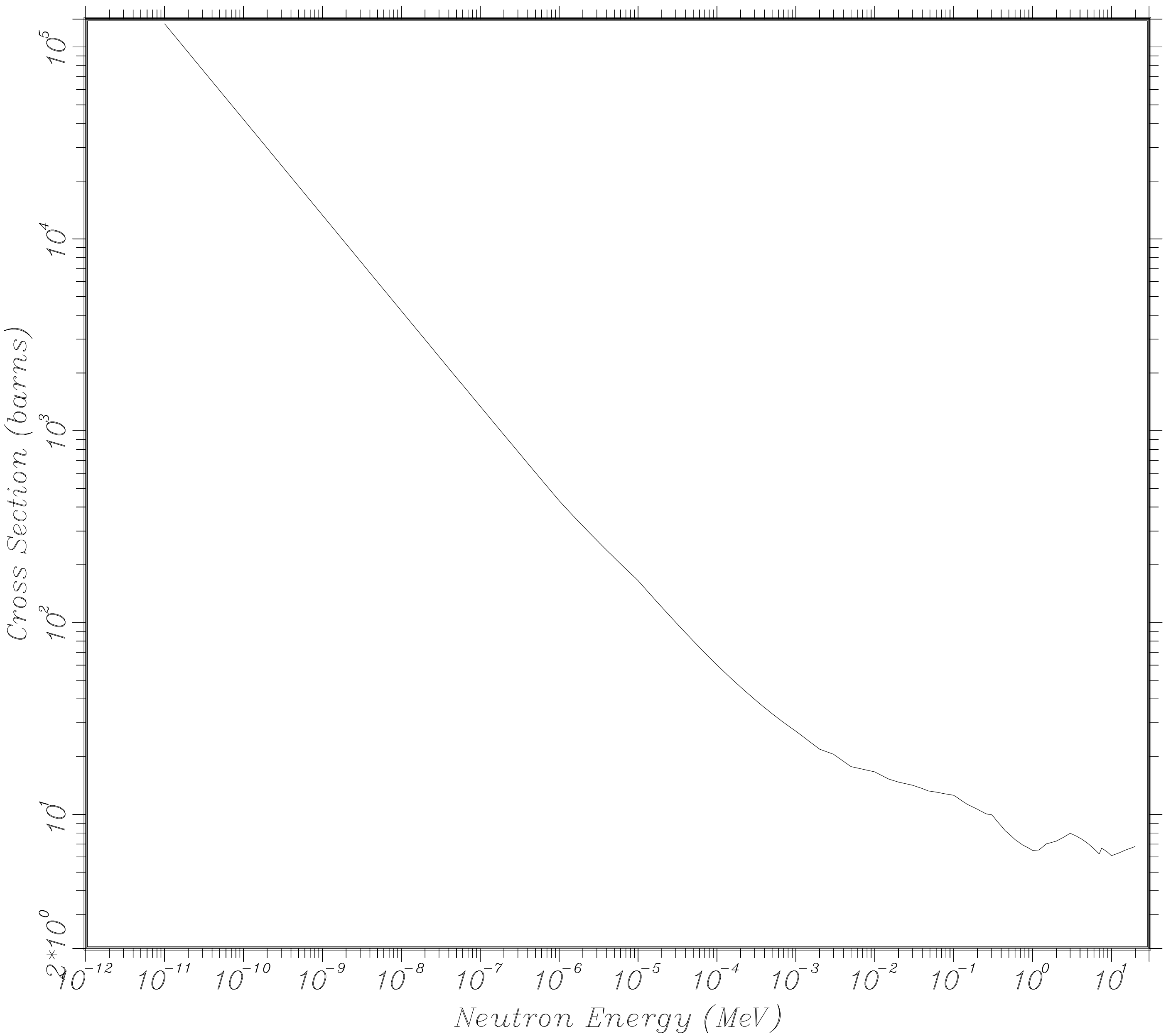
Pu - 236

From ENDF602

MT = 1

TOTAL

Figure 5: Total Cross Section for Pu–237



09/23/96

ZAID = 94237.60C

Pu – 237

From ENDF602

MT = 1

TOTAL